NON-EQUILIBRIUM MODELING OF COMPLEX TURBULENT FLOWS

Charles G. Speziale

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ABSTRACT

The non-equilibrium modeling of complex turbulent flows is considered from a theoretical standpoint. Both two-equation models and full second-order closures are considered. Non-equilibrium two-equation models can be obtained via a regularization scheme based on a Pade' approximation. Second-order closures that are extended to non-equilibrium flows are obtained in the same fashion. Applications to rapidly distorted flows – including homogeneous shear flow and homogeneous plane strain turbulence – are considered. The prospects for future research are discussed in detail.

1. INTRODUCTION

Much research has been accomplished during the past five years. All of the proposed work has been completed. It was proposed to develop non-equilibrium pressure-strain models as well as to incorporate non-equilibrium vortex stretching and anisotropic dissipation. During the last two years, a new methodology for large-eddy simulations (LES) was to be developed. The starting point of this research was to develop explicit algebraic stress models that are suitable for non-equilibrium turbulent flows. Explicit algebraic stress models, which are in the form of anisotropic eddy viscosity models, are normally obtained from full second-order closures in the limit of equilibrium turbulent flows under certain specific assumptions. The fact that explicit algebraic stress models – which are single-valued – are derived in two ways was first recognized. Either the ratio of production to dissipation can be set equal to a constant in the coefficients or the consistency condition – with its associated cubic equation – can be solved. When the ratio of production to dissipation is set equal to a constant a singularity arises. This necessitates the use of a regularization procedure that removes the singularity. Far from being a deficiency, this regularization has turned out to be a virtue. By using a two-sided Padé approximation, it is possible to develop models that are indistinguishable from the original model in equilibrium turbulent flows where it formally applies but then the model applies to the far from equilibrium rapid distortion case which is normally approximated by Rapid Distortion Theory (RDT). Thus, non-equilibrium turbulent flows can be described by a regularization based on a Padé approximation. The results collapsed homogeneous shear flow in the RDT limit which is far from equilibrium. Plane strain turbulence was also considered with success. This was done while maintaining agreement for equilibrium turbulent flows by starting with an explicit algebraic stress model that does well for such flows (this is easy to accomplish since explicit algebraic stress models formally apply in the equilibrium limit for which the regularization is negligible). By using this approach, a whole new way of developing second-order closure models, by a relaxation time approximation was presented. It was systematically and fully shown that second-order closure models can be developed by conducting a relaxation time approximation of the non-equilibrium algebraic stress models developed herein. By using the form suggested by this approach for the rapid pressure-strain correlation, a non-equilibrium second-order closure was developed which is of the traditional form except that strain-dependent coefficients are

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used. For near equilibrium turbulent flows it collapses to the SSG model – a second-order closure which does well for such flows; it is able to describe non-equilibrium turbulent flows in the rapid distortion limit: both homogeneous shear flow and plane strain turbulence – the two most basic benchmark flows – are well described in the RDT limit as will be shown. Thus, a new methodology is at hand to develop non-equilibrium second-order closure models. Since, the non-equilibrium features are manifested through strain-dependent coefficients, this approach is easy to implement in any computer codes that implement traditional second-order closure models.

An entirely new approach based on a combined time-dependent RANS/LES approach was developed based on this methodology in the last two years. This approach is only slightly more expensive to implement than traditional approaches. It is critical that these two approaches be combined since the best that one can currently do at the extremely high Reynolds numbers that occur in many flows of technological interest is a time-dependent Reynolds-averaged Navier-Stokes (RANS) calculation. Subgrid scale models were developed that go continuously to Reynolds stress models in the coarse mesh/infinite Reynolds number limit. This was accomplished by parameterizing these models by the ratio of the grid size to the Kolmogorov length scale that determines how well resolved a computation is in the numerical simulation of turbulence and is the proper parameter to use. A RANS calculation is done in parallel to get an estimate of the Kolmogorov length scale from the dissipation rate equation. Furthermore, the subgrid scale models have a dependence on rotational strains which can be extremely important. Rotations can severely impede the cascade leading to subgrid scale models that must be substantially less dissipative. The initial tests of this idea in the boundary layer were quite successful so further tests were conducted. With these ideas, it is possible to conduct an LES through transition and for an extremely high Reynolds number boundary layer a RANS calculation is automatically recovered. This is quite exciting and holds the potential to achieve the long held dream of continuously going from an LES to a RANS computation.

2. RESEARCH ACCOMPLISHED

For two-dimensional mean turbulent flows, explicit algebraic stress models – obtained from second-order closures by integrity bases techniques – take the simplified form (see

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Gatski and Speziale 1993):

$$
\tau_{ij} = \frac{2}{3} K \delta_{ij} - \frac{3}{3 - 2\eta^2 + 6\xi^2} \left[\alpha_1 \frac{K^2}{\varepsilon} \overline{S}_{ij} \right.
$$

$$
+ \alpha_2 \frac{K^3}{\varepsilon^2} (\overline{S}_{ik} \overline{\omega}_{kj} + \overline{S}_{jk} \overline{\omega}_{ki}) \tag{1}
$$

$$
\left. - \alpha_3 \frac{K^3}{\varepsilon^2} \left(\overline{S}_{ik} \overline{S}_{kj} - \frac{1}{3} \overline{S}_{kl} \overline{S}_{kl} \delta_{ij} \right) \right]
$$

where

$$
\alpha_1 = \left(\frac{4}{3} - C_2 \right) g, \quad \alpha_2 = \frac{1}{2} \left(\frac{4}{3} - C_2 \right) (2 - C_4) g^2
$$

$$
\alpha_3 = \left(\frac{4}{3} - C_2 \right) (2 - C_3) g^2, \quad g = \left(\frac{1}{2} C_1 + \frac{\mathcal{P}}{\varepsilon} - 1 \right)^{-1}
$$

$$
\eta = \frac{1}{2} \frac{\alpha_3}{\alpha_1} \frac{K}{\varepsilon} (\overline{S}_{ij} \overline{S}_{ij})^{1/2}, \quad \xi = \frac{\alpha_2}{\alpha_1} \frac{K}{\varepsilon} (\overline{\omega}_{ij} \overline{\omega}_{ij})^{1/2} \tag{2}
$$

and where $\overline{S}_{ij}$ and $\overline{\omega}_{ij}$ are the mean rate of strain and mean vorticity tensors with the constants $C_1 - C_4$ provided by the pressure-strain model; C_1 is the Rotta constant and K and ε are the turbulent kinetic energy and dissipation rate. In (2), the ratio of production to dissipation $\mathcal{P}/\varepsilon$ that appears in the coefficient g can be approximated by its constant equilibrium value (a value of one has been recently chosen with success). The explicit solution for τ_{ij} given in (1) formally constitutes an anisotropic eddy viscosity model with *strain-dependent* coefficients (earlier anisotropic eddy viscosity models erroneously had constant coefficients; see Yoshizawa 1984, Speziale 1987, and Rubinstein and Barton 1990). As demonstrated by Gatski and Speziale (1993) and first derived by Pope (1975), the explicit ASM given in (1) yields results that are virtually indistinguishable from the corresponding full second-order closure for turbulent flows that are close to equilibrium. While (1) provides an excellent description of near-equilibrium turbulent flows, it is rather obvious that it fails for turbulent flows that are far from equilibrium where it is possible for a singularity to arise (for sufficiently large values of η, the denominator $3 - 2\eta^2 + 6\xi^2$ can vanish; a singularity, thus, arises when $\mathcal{P}/\varepsilon$ is set to a constant value). Since (1) is the explicit solution to the traditional algebraic stress models, it is now clear why such models have, in many applications to complex turbulent flows, given rise to divergent computations (see Gatski and Speziale 1993). By utilizing the fact that for equilibrium turbulent flows η is substantially less than

one, Gatski and Speziale (1993) introduced the approximation

$$\frac{3}{3 - 2\eta^2 + 6\xi^2} \approx \frac{3(1 + \eta^2)}{3 + \eta^2 + 6\xi^2\eta^2 + 6\xi^2} \tag{3}$$

and it is a formally valid approximation in equilibrium which is based on a one-sided Taylor expansion and removes the singularity. The use of (3) allows the model to be computable through highly non-equilibrium regimes. While (3) makes the model well behaved in far from equilibrium turbulent flows, it is not expected to have any predictive capabilities therein. This deficiency can be overcome by implementing a formal two-sided Padé approximation that establishes some limited consistency with Rapid Distortion Theory (RDT) which applies to strongly strained turbulent flows that are far from equilibrium. While (1) provides an excellent description of near-equilibrium turbulent flows, it is rather obvious that it fails for turbulent flows that are far from equilibrium where it is possible for a singularity to arise as discussed before (for sufficiently large values of η, the denominator $3 - 2\eta^2 + 6\xi^2$ can vanish when $\mathcal{P}/\varepsilon$ is set to a constant). Since (1) is the explicit solution to the traditional algebraic stress models, it is now clear why such models have, in many applications to complex turbulent flows, given rise to to non-convergent computations (this was discussed in more detail in Speziale 1997a). By utilizing the fact that for equilibrium turbulent flows η is substantially less than one, Gatski and Speziale (1993) introduced the approximation described in (3) which removes the singularity. The use of (3) allows the model to be computable through highly non-equilibrium regimes. While (3) makes the model well behaved in far from equilibrium flows, it would not be expected to have any predictive capabilities therein. This deficiency can be overcome as discussed above by implementing a formal two-sided Padé approximation that establishes some limited consistency with Rapid Distortion Theory (RDT) which applies to strongly strained turbulent flows that are far from equilibrium.

Homogeneous shear flow will be the primary focus of our attention where the mean velocity gradient tensor takes the form

$$\partial \overline{v}_i / \partial x_j = S\delta_{i1}\delta_{j2}. \tag{4}$$

Plane strain turbulence will also be considered. In (4), S is a constant shear rate that is applied uniformly starting at time $t = 0$, to an initially isotropic turbulence with turbulent kinetic energy K_0 and dissipation rate ε_0. For strongly sheared homogeneous turbulence

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– where $SK_0/\varepsilon_0 \gg 1$ – the RDT solution constitutes an excellent approximation for early times (i.e., at least for some significant fraction of an eddy turnover time). The transport equation for the turbulent kinetic energy – which is obtained by contracting the Reynolds stress transport equation – takes the form

$$\dot{K} = \mathcal{P} - \varepsilon \tag{5}$$

in homogeneous shear flow, where $\mathcal{P} = -\tau_{12}S$ is the turbulence production. In the RDT limit, where $SK_0/\varepsilon_0 \to \infty$, and the dissipation rate in (5) can be neglected leading to the dimensionless form

$$\dot{K}^* = -\frac{\tau_{12}}{K_0} \tag{6}$$

where $K^* \equiv K/K_0$ and $\dot{K}^*$ is its derivative with respect to the dimensionless time, $t^* \equiv St$. The long time asymptotic solution to the RDT equations has been obtained analytically (see Rogers 1991). It is given by

$$\frac{\tau_{12}}{K_0} = -2ln2 \tag{7}$$

$$K^* = (2ln2)t^* \tag{8}$$

$$b_{11} = \frac{2}{3}, \quad b_{22} = b_{33} = -\frac{1}{3} \tag{9}$$

in the limit as $t^* \to \infty$. This RDT solution corresponds to a linear (algebraic) growth of the turbulent kinetic energy with an associated one component state of turbulence as exemplified by (9).

The long-time asymptotic solution for RDT is not of value, in and of itself, since the assumptions underlying the RDT approximation break down for large times. However, when combined with (6) – (9) it does provide us with the following useful information: (a) the RDT solution for τ_{12}/K_0 starts from zero and remains bounded and of order one, and (b) the normal Reynolds stress anisotropies try to approach, from zero, a one component state where $b_{11} = 2/3$, $b_{22} = -1/3$ and $b_{33} = -1/3$. DNS results of Lee, et al. (1990) indicate that this happens in a fraction of an eddy turnover time. This places a major constraint on the explicit ASM, given in (1), which can be re-written in the form

$$\tau_{ij} = \frac{2}{3}K\delta_{ij} - \alpha_1^*\frac{K^2}{\varepsilon}\overline{S}_{ij} - \alpha_2^*\frac{K^3}{\varepsilon^2}(\overline{S}_{ik}\overline{\omega}_{kj}$$

$$+\overline{S}_{jk}\overline{\omega}_{ki}) + \alpha_3^*\frac{K^3}{\varepsilon^2}\left(\overline{S}_{ik}\overline{S}_{kj} - \frac{1}{3}\overline{S}_{kl}\overline{S}_{kl}\delta_{ij}\right) \tag{10}$$

where

$$\alpha_i^* = \alpha_i \left(\frac{3}{3 - 2\eta^2 + 6\xi^2} \right)$$

for $i = 1, 2, 3$. From (8), it is clear that

$$\frac{\tau_{12}}{K_0} = -\frac{1}{2}\alpha_1^* \left(\frac{SK}{\varepsilon} \right) \left(\frac{K}{K_0} \right). \tag{11}$$

Since, in the short-time RDT solution, $SK/\varepsilon \to \infty$ while K/K_0 remains of order one, it is obvious that

$$\alpha_1^* \sim \frac{1}{\eta} \tag{12}$$

where we have made use of the fact that $\eta \propto \xi \propto SK/\varepsilon$ in homogeneous shear flow. It is clear that the equilibrium model – encompassed by (1) – violates this constraint. This problem can be remedied via a Padé approximation whereby (1) is replaced by a regularized expression that is approximately equal to (1) for the near-equilibrium case (where $\eta < 1$) but has the correct asymptotic behavior, given above, for $\eta \gg 1$. One such approximation, which is accurate to $O(\eta^4)$, is as follows (see Speziale and Xu 1996):

$$\alpha_1^* = \frac{(1 + 2\xi^2)(1 + 6\eta^5) + \frac{5}{3}\eta^2}{(1 + 2\xi^2)(1 + 2\xi^2 + \eta^2 + 6\beta_1\eta^6)}\alpha_1 \tag{13}$$

where β_1 is an arbitrary constant. Equation (13) is regular for all values of η and ξ. It yields results that are within one percent of (1) for near-equilibrium turbulent flows (where the latter is valid) and has the correct asymptotic behavior of $\alpha_1^* \sim 1/\eta$ for $\eta \gg 1$. The equations given above suggest that β_1 is in the range of 5 - 10.

While the regularized expression (3), derived by Gatski and Speziale (1993), is asymptotically consistent for the b_{11}, b_{22} and b_{33} components, it does not yield the correct tendency to a one component state in the RDT limit. This can be remedied by the alternative form, obtained by a Padé approximation that is accurate to $O(\eta^4)$ (see Speziale and Xu 1996):

$$\alpha_i^* = \frac{(1 + 2\xi^2)(1 + \eta^4) + \frac{2}{3}\eta^2}{(1 + 2\xi^2)(1 + 2\xi^2 + \beta_i\eta^6)}\alpha_i \tag{14}$$

where β_i is an arbitrary constant ($i = 2, 3$). Equation (14) represents an excellent approximation to (1) for near-equilibrium turbulent flows. It is regular for all values of η and ξ, has the correct asymptotic behavior for $\eta \gg 1$ and, for values of β_2 and β_3 of approximately 5, predicts an approach to a one component state consistent with RDT of homogeneous

shear flow. The constants β_1, β_2 and β_3 are approximately 7, 6, and 4. The two-equation model can be integrated to a solid boundary with no wall damping (see Speziale and Abid 1995). By including a vortex stretching term, the model can be further regularized and a value of one can be chosen for the ratio of production to dissipation (see Abid and Speziale 1996). Furthermore, the inclusion of anisotropic dissipation can be useful in describing more turbulence physics by a simple means (see Speziale and Gatski 1997 and Xu and Speziale 1996). This, furthermore, completes the proposed research.

Second-order closures that are suitable for non-equilibrium turbulent flows can then be obtained by conducting a relaxation time approximation around the non-equilibrium extension of the explicit ASM. The idea of obtaining second-order closures by a relaxation time approximation around an equilibrium algebraic model is probably first attributable to Saffman (1977) (this stood in contrast with the more commonly adopted approach of directly modeling the higher-order correlations that appear in the Reynolds stress transport equation which was popular even before Launder, Reece and Rodi 1975). However, Saffman (1977) implemented this relaxation time approximation about a simple, nonlinear algebraic representation for the Reynolds stress tensor. In contrast to this approach, we have implemented a relaxation time approximation about the non-equilibrium extension of the explicit ASM written in terms of the Reynolds stress anisotropy tensor (in strained homogeneous turbulent flows, it is only the Reynolds stress anisotropy that equilibrates; the Reynolds stresses grow exponentially). Hence, we have proposed the relaxation model

$$\dot{b}_{ij} = -C_R \frac{\varepsilon}{K}(b_{ij} - b_{ij}^{E^*}) \tag{15}$$

where

$$b_{ij}^{E^*} = -\frac{1}{2}\alpha_1^* \frac{K}{\varepsilon}\overline{S}_{ij} - \frac{1}{2}\alpha_2^* \frac{K^2}{\varepsilon^2}(\overline{S}_{ik}\overline{\omega}_{kj} + \overline{S}_{jk}\overline{\omega}_{ki})$$
$$+ \frac{1}{2}\alpha_3^* \frac{K^2}{\varepsilon^2}\left(\overline{S}_{ik}\overline{S}_{kj} - \frac{1}{3}\overline{S}_{kl}\overline{S}_{kl}\delta_{ij}\right) \tag{16}$$

is the non-equilibrium extension of (1), written in terms of the anisotropy tensor, with $\alpha_1^* - \alpha_3^*$ given by their non-equilibrium forms (13) – (14). In (15), C_R is a dimensionless relaxation coefficient. Consistency with the Crow (1968) constraint requires that:

$$C_R = \frac{8}{15}\left(\frac{3 - 2\eta^2}{3\alpha_1}\right) \tag{17}$$

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in an initially isotropic turbulence subjected to a mild strain. Of course, for strongly strained turbulent flows, (17) must be regularized. One preliminary form that is being considered is given by

$$C_R = \frac{8}{15\alpha_1} \frac{1 + \eta^2 + 6\beta_1\eta^6}{1 + \frac{5}{3}\eta^2 + 6\eta^5}.$$ (18)

When (15) is rearranged into a transport equation for the Reynolds stress tensor, it yields a model that differs from the traditional models in a notable way: the rapid pressure-strain correlation depends linearly on the anisotropy tensor, but depends nonlinearly on the invariants of the rotational and irrotational strain rates, i.e.,

$$M_{ijkl} = M_{ijkl}(\mathbf{b}; \eta, \xi)$$ (19)

to the lowest order. A preliminary form is currently being considered and it appears to lead to a considerable improvement.

In order to establish a benchmark for the performance of the models in near-equilibrium turbulent flows, we will first consider the test case of Bardina, Ferziger and Reynolds (1983) for homogeneous shear flow. This corresponds to an initial condition of $SK_0/\varepsilon_0 = 3.38$ which is not far removed from the equilibrium value of SK/ε which is in the range of 5 to 6. In Figure 1, the time evolution of the turbulent kinetic energy K^* obtained from the SSG model and the explicit ASM based on the SSG model are compared with the large-eddy simulation (LES) results of Bardina, Ferziger and Reynolds (1983). It is clear from these results that both the SSG model (see Speziale, Sarkar and Gatski 1991) and its equilibrium ASM do an excellent job of capturing the LES results since they are close to equilibrium. This is not so of the standard $K - \varepsilon$ model of Launder and Spalding (1974) which has a growth rate that is somewhat too large.

Now we will consider the far from equilibrium test case where $SK_0/\varepsilon_0 = 50$; for this strongly sheared case, RDT constitutes a good approximation for early times. In Figure 2, the time evolution of the turbulent kinetic energy predicted by the models is compared with the RDT solution (Rogers 1991 and Rogers, private communication). It is clear from these results that none of the models are able to predict the correct trend (DNS results have tended to indicate that, for this case, RDT is a good approximation until $St = 12$). The interesting point here is that the SSG second-order closure predicts too large a growth rate whereas the explicit ASM based on the SSG model yields a growth rate that is far too low. Here,

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the former problem arises from the fact that traditional pressure-strain models (see Speziale 1996) do not apply to turbulent flows that are far from equilibrium; the latter problem is due to the fact that the regularization procedure used earlier by Gatski and Speziale (1993) does not apply to turbulent flows that are strongly strained (the eddy viscosity $\nu_T \sim 1/\eta^2$ instead of like $1/\eta$ which explains the low growth rate). On the other hand, the standard $K - \varepsilon$ model renders $\nu_T \sim 0(1)$ which explains its enormous growth rate (the standard $K - \varepsilon$ model erroneously predicts that $\dot{K}^* \to \infty$ as $\eta \to \infty$). We will present results for the new non-equilibrium model developed herein. The results correspond to the choice of constants

$$\beta_1 = 7.0, \quad \beta_2 = 6.3, \quad \beta_3 = 4.0 \tag{20}$$

in the regularized coefficients $\alpha_1^* - \alpha_3^*$ given in (13)-(14). The predictions of the new explicit ASM for the time evolution of the turbulent kinetic energy are compared in Figure 3 with the RDT solution. With this new non-equilibrium extension, the results are remarkably improved. It is not even necessary to introduce the relaxation time approximation (from (18), the relaxation coefficient is large for this case, rendering its effect small on K^*). In Figure 4, the time evolution of the normal components of the Reynolds stress anisotropy tensor obtained from the new relaxation model (for $SK_0/\varepsilon_0 = 50$) are compared with RDT as well as with the predictions of the SSG second-order closure. Here again, the new model yields a substantial improvement, rendering results that are more properly in line with an approach to a one-component state predicted by RDT. Similarly good results have been obtained for plane strain turbulence in the RDT limit as shown in Figures 5 – 6 where the growth rate of the equilibrium model is far too large. It should be mentioned, however, that these results could change with time due to the fact that the relaxation coefficient C_R could change (there are ambiguities that remain in what regularization procedure is implemented and how $\mathcal{P}/\varepsilon$ is chosen in α_1; for now we are taking it to be one which seems to yield good results). This, however, is not important; the important thing is the ideas and the fact that a model that can currently be used has been developed.

Using these ideas, a non-equilibrium second-order closure model has been developed of the traditional form except that it has strain-dependent coefficients. This has been based on (19) which says that the coefficients of the rapid pressure-strain are strain dependent in a nonlinear way. A generalization to the SSG model has been obtained. The SSG model

assumes the quasi-linear form for the pressure-strain correlation (see Speziale, Sarkar and Gatski 1991):

$$
\begin{aligned}
\Pi_{ij} &= -(C_1 \varepsilon + C_1^* \mathcal{P}) b_{ij} + C_2 \varepsilon \left(b_{ik} b_{kj} - \frac{1}{3} b_{k\ell} b_{k\ell} \delta_{ij} \right) \\
&\quad + (C_3 - C_3^* II_b^{1/2}) K \overline{S}_{ij} + C_4 K \left(b_{ik} \overline{S}_{jk} + b_{jk} \overline{S}_{ik} \right. \\
&\quad \left. - \frac{2}{3} b_{k\ell} \overline{S}_{k\ell} \delta_{ij} \right) + C_5 K (b_{ik} \overline{\omega}_{jk} + b_{jk} \overline{\omega}_{ik})
\end{aligned}
\tag{21}
$$

where

$$
C_1 = 3.4, \ C_1^* = 1.80, \ C_2 = 4.2, \ C_3 = \frac{4}{5}
$$

$$
C_3^* = 1.30, \ C_4 = 1.25, \ C_5 = 0.40, \ II_b = b_{ij} b_{ij}.
$$

The Launder, Reece and Rodi (1975) model is recovered as a special case of the SSG model when

$$
C_1 = 3.0, \ C_1^* = 0, \ C_2 = 0, \ C_3 = \frac{4}{5}, \ C_3^* = 0,
$$

$$
C_4 = 1.75, \ C_5 = 1.31.
$$

Hence, the SSG model can be easily implemented in any computer code that makes use of the Launder, Reece and Rodi model (the same will be true of the non-equilibrium extension of the SSG model to be presented). The SSG model can then be extended to non-equilibrium turbulent flows – by making use of (19) – through a heuristic Padé approximation of the coefficients which also builds in agreement with the RDT solution for plane strain as well as homogeneous shear flow. The coefficients in this model take the form:

$$
C_1 = 3.4, \quad C_2 = 4.2, \quad C_3 = 0.8
$$

$$
C_1^* = \frac{1.8 + 0.225 \eta^6}{1 + 0.0625 \eta^6 + 0.5 \xi^8} \quad C_3^* = \frac{1.3 + 8.84 \eta^8}{1 + 9.02 \eta^8}
$$

$$
C_4 = \frac{1.25 + 6.33 \eta^6}{1 + 1.52 \eta^6 + 0.1 \xi^7}, \quad C_5 = \frac{0.4 + 0.114 \eta^6}{1 + 0.285 \eta^6 + 0.5 \xi^8}.
$$

This yields results indistinguishable from the SSG model for equilibrium turbulent flows where $\eta, \xi < 1$ (for homogeneous shear flow in equilibrium, $\eta \approx 0.4$ and $\xi \approx 0.7$). But in the non-equilibrium rapid distortion limit, where $\eta, \xi \to \infty$, considerably different values of the coefficients are obtained. This is consistent with the findings of Reynolds (*Private Communication*) and Reynolds (1987) who found that a different form for $\mathcal{M}_{ijkl}$ was needed

for the rapid distortion limit compared to equilibrium turbulent flows. The way that this can be achieved is to let $\mathcal{M}_{ijkl}$ be a function of η, ζ as in (19). In Figures 7 – 10 (for $SK_0/\varepsilon_0 = 100$ and $\Gamma K_0/\varepsilon_0 = 50$), it is shown how this leads to a much better description of homogeneous shear flow and plane strain turbulence for a wide range of shear and strain rates that includes the rapid distortion limit (the model is approximately equal to its equilibrium form in that limit where it does well as shown in Speziale, Sarkar and Gatski 1991). The growth rate of the turbulent kinetic energy and the Reynolds stress anisotropies are in considerable error for the equilibrium model as compared to the new non-equilibrium model which performs well in near equilibrium cases as well as the RDT cases considered.

Results will also be presented for the new approach to LES which has been discussed in Speziale (1997b, 1998). Some preliminary LES results will be shown for the developing turbulent boundary layer — integrated through transition. First, a more detailed discussion of this new approach will be provided. The methodology we are proposing for large-eddy simulations has subgrid scale stress models that are of the following form:

$$\tau_{ij} = [1 - exp(-\beta\Delta/L_K)]^n \alpha_1 f(\eta, \zeta) \frac{K^2}{\varepsilon} \overline{S}_{ij} + anisotropic\ eddy\ viscosity\ terms. \quad (22)$$

Thus, the subgrid scale stress is written partially in terms of filtered fields. Here, an overbar represents a *standard* filter, $\eta \propto (\overline{S}_{ij}\overline{S}_{ij})^{1/2}K/\varepsilon$, $\zeta \propto (\overline{W}_{ij}\overline{W}_{ij})^{1/2}K/\varepsilon$ where $\overline{S}_{ij}$ and $\overline{W}_{ij}$ are the filtered rate of strain and vorticity tensors, Δ is the computational mesh size, and L_K is the Kolmogorov length scale (α_1 and β are constants; α_1 is obtained from a Reynolds stress model along with the function f). Here, K and ε represent the Reynolds-averaged turbulent kinetic energy and dissipation rate obtained from a *Reynolds stress calculation* with the two-equation models discussed earlier. These have to be obtained anyway in order to get an estimate of the Kolmogorov length scale L_K. Since, the Kolmogorov length scale $L_K = \nu^{3/4}/\varepsilon^{1/4}$ (where ν is the kinematic viscosity), the dissipation rate only has to be estimated to within 50% with the modeled dissipation rate equation to get a good estimate of the Kolmogorov length scale (the dissipation rate is raised to the 1/4 power). Thus, this methodology requires that a RANS calculation be done in parallel with the LES. This will, in most circumstances, only add at most 10% to the computational expense. Here, we parameterize the model in terms of the Reynolds-averaged turbulent kinetic energy and dissipation rate since the subgrid scale turbulent kinetic energy and dissipation rate can vary

too much locally. We have written this model before in the shorthand notation as

$$\tau_{ij} = [1 - exp(-\beta\Delta/L_K)]^n R_{ij}$$

where R_{ij} is a Reynolds stress model that is written partially in terms of filtered fields. An explicit algebraic stress model is used for this purpose as given above.

On the other hand, the Smagorinsky model takes the form:

$$\tau_{ij} = C_s^2\Delta^2(2\overline{S}_{ij}\overline{S}_{ij})^{1/2}\overline{S}_{ij}$$

where C_s is the Smagorinsky constant (see Smagorinsky 1963). This has several deficiencies in comparison to our proposed approach which can be summarized as follows:

(1) The Smagorinsky constant is not in reality a constant. It can vary by as much as a factor of two or three from flow to flow. In our approach this variation is parameterized by the Reynolds-averaged turbulent kinetic energy and dissipation rate that are obtained from a RANS calculation. These are needed anyhow to get an estimate of the Kolmogorov length scale which is an integral part of our new methodology. We decidedly *do not* use the subgrid scale turbulent kinetic energy and dissipation rate for this purpose since they can vary too much. The variation of the constants can probably be adequately parameterized by the mean turbulent fields K and ε.

(2) The Smagorinsky model *does not* depend on the rotational strains through the invariant ξ and, furthermore, has the wrong dependence on the irrotational strain rate invariant η. For Reynolds stress models in equilibrium (see Gatski and Speziale 1993)

$$f(\eta, \xi) = \frac{3}{3 - 2\eta^2 + 6\xi^2}.$$

where we use regularized versions of this representation that avoids the singularity. The choice of $f(\eta, \xi) \propto \eta$ in the Smagorinsky model is simply wrong and probably contributes to the Smagorinsky constant changing so much. Furthermore, we have an additional dependence on rotational strains through ξ and the anisotropic eddy viscosity term

$$[1 - exp(-\beta\Delta/L_K)]^n[\alpha_2\frac{K^3}{\varepsilon^2}f(\eta, \xi)(\overline{W}_{ik}\overline{S}_{kj} + \overline{W}_{jk}\overline{S}_{ki})$$

$$+\alpha_3\frac{K^3}{\varepsilon^2}f(\eta, \xi)(\overline{S}_{ik}\overline{S}_{kj} - \frac{1}{3}\overline{S}_{kl}\overline{S}_{kl}\delta_{ij}) \tag{23}$$

where α_2 and *alpha3* are constants. This term accounts for backscatter effects.

(3) The dependence on the computational mesh size Δ in our model is through the dimensionless ratio Δ/L_K. *What determines how well a computation is resolved is whether or not the grid size is small (or large) compared to the Kolmogorov length scale.* The dimensional dependence on Δ in the Smagorinsky model is simply incorrect. Since we use a filter that yields a minimum contamination of the large scales (this is guaranteed by any filter with a small compact support on a 128^3 mesh), a state-of-the-art Reynolds stress model is recovered in the coarse mesh/infinite Reynolds number limit as Δ/L_K tends to infinity ($L_K \equiv R_t^{-3/4} K^{3/2}/\varepsilon$ where R_t is the turbulence Reynolds number). On the other hand, the Smagorinsky model goes to a badly calibrated Reynolds stress model in the coarse mesh limit (the same is true of the dynamic subgrid scale model). Hence, with this methodology it is possible to achieve the long held dream of going continuously from a large-eddy simulation to a Reynolds stress calculation as the mesh becomes coarse or the Reynolds number becomes extremely large. In wall-bounded geometries, the best we can currently do – at extremely high Reynolds numbers – is a Reynolds stress calculation. Of course, as with the Smagorinsky model, the subgrid scale stress $\tau_{ij} \to 0$ in our model as $\Delta \to 0$ allowing a DNS to be recovered. However, here the dependence is properly parameterized by the dimensionless ratio of the mesh size to the Kolmogorov length scale Δ/L_K.

The model has now been calibrated ($\beta \approx 0.001$, $n \approx 1$). In our opinion, this proposed approach is far superior to the Smagorinsky model or the dynamic subgrid scale model and holds great promise for making a major impact on large-eddy simulations.

Computations have been conducted by H. Fasel and his group at the University of Arizona initially using an empirically based ramp function — that depends explicitly on the momentum thickness Reynolds number and the mesh size with a simple eddy viscosity model — as a preliminary test of the ideas in this new combined LES and time-dependent RANS approach. In Figure 11, the spanwise vorticity obtained from the LES is shown which compares favorably with the corresponding results obtained from DNS. It is clear that the subgrid scale model allows the LES to pick up the pertinent flow structures and to be integrated through transition (laminar – turbulent flow). The ramp function, which forms a central part of this approach, allows the eddy viscosity to gradually turn on as the flow becomes turbulent. In this regard, the corresponding eddy viscosity is displayed in Figure 12. These

preliminary results are extremely encouraging and demonstrate the potential of this new approach for a combined LES and time-dependent RANS methodology.

3. CONCLUSION

It was shown that non-equilibrium extensions of explicit algebraic stress models can be obtained by a two-sided Padé approximation. Explicit algebraic stress models are convenient because they are in the form of anisotropic eddy viscosity models. In the equilibrium limit they yield results that are indistinguishable from full second-order closures on which they are based. When formulated this, way both explicit algebraic stress models and full second-order closures can be obtained that can describe the far from equilibrium RDT cases of homogeneous shear flow and plane strain turbulence as well as benchmark equilibrium flows. Traditional models fail abysmally on these test cases which are basic. A new combined LES/time-dependent RANS capability was developed using these developments in Reynolds stress modeling. Subgrid scale models were developed that go continuously to state-of-the-art Reynolds stress models in the coarse mesh/infinite Reynolds number limit. They are more properly parameterized by the dimensionless ratio of the computational grid size to the Kolmogorov length scale – the parameter that determines how well resolved a computation is in the numerical simulation of turbulence. This appears to allow the long held dream of going continuously from an LES to a RANS to be achieved. Preliminary numerical tests on the turbulent boundary layer are quite encouraging.

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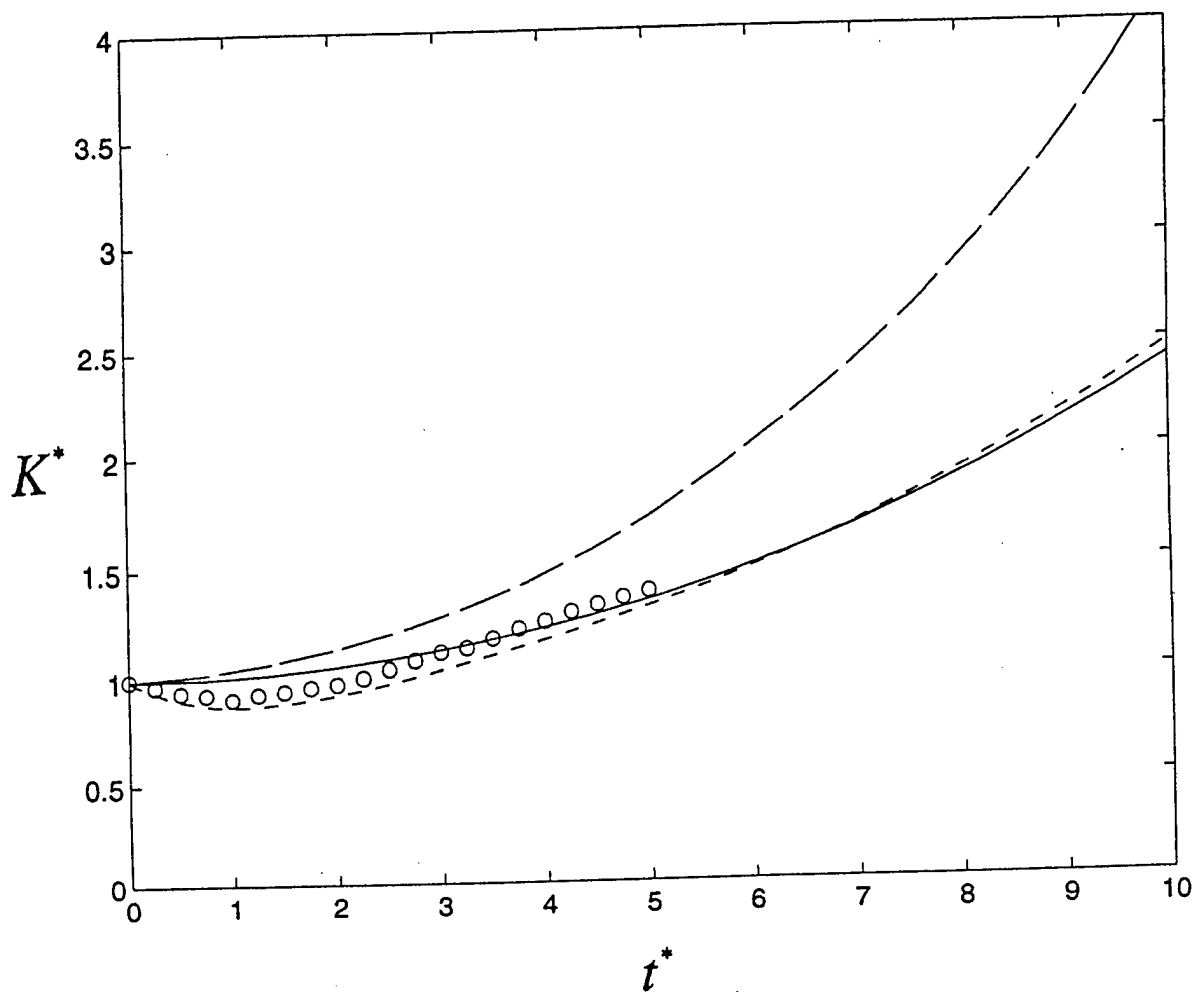
(Several other Articles are to appear)

Figure 1. Time evolution of the turbulent kinetic energy in homogeneous shear flow: Comparison of model predictions with the large-eddy simulation (LES) of Bardina, Ferziger and Reynolds (1983) for $SK_0 / \varepsilon_0 = 3.38$. (- - -) SSG Model; (— —) $K - \varepsilon$ Model; (——) Explicit ASM of Gatski & Speziale (1993) ; (o) LES.
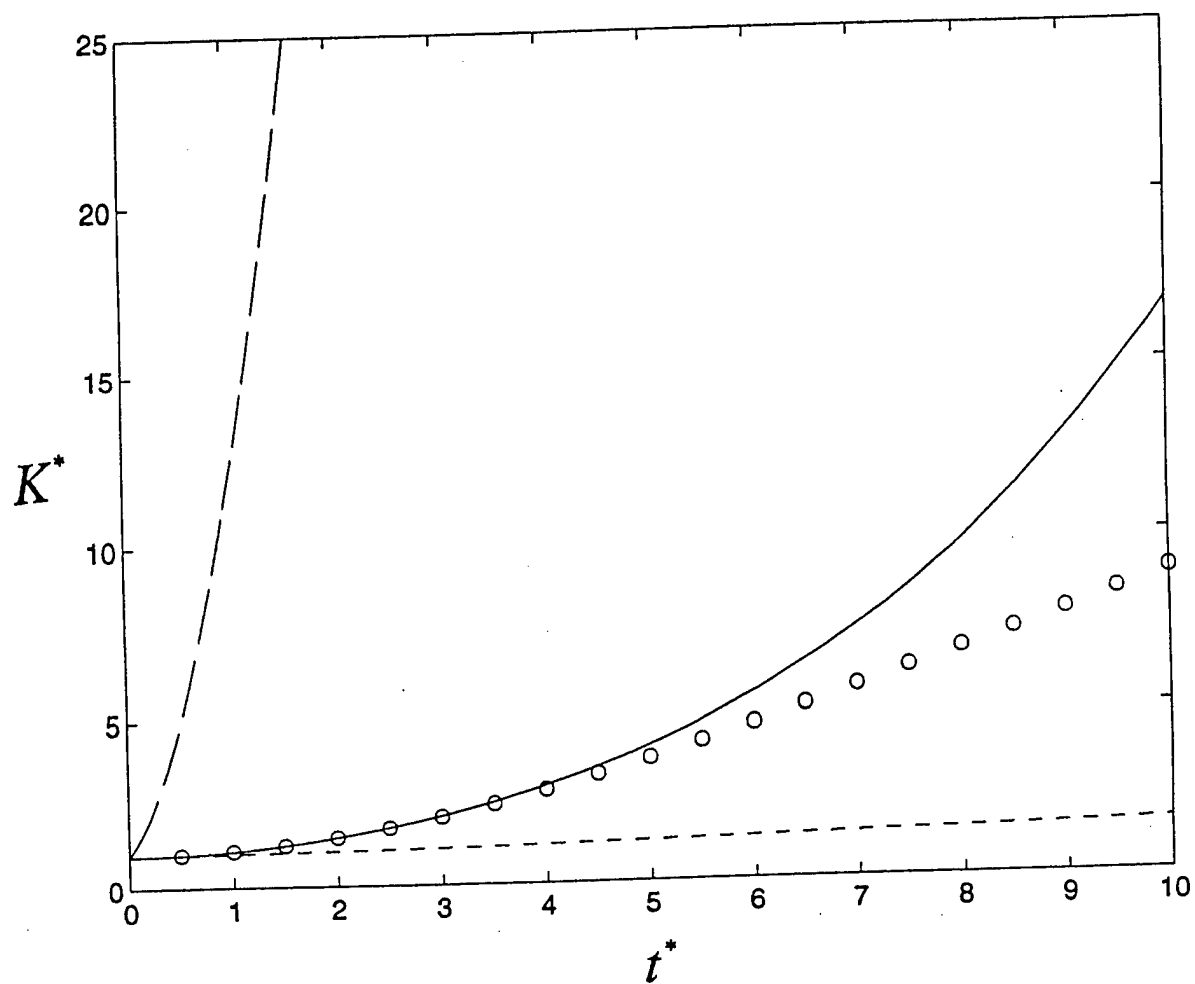
Figure 2. Time evolution of the turbulent kinetic energy in homogeneous shear flow: Comparison of model predictions for $SK_0 / \varepsilon_0 = 50$ with Rapid Distortion Theory (RDT). (——) SSG Model; (— —) $K - \varepsilon$ Model; (- - -) Explicit ASM of Gatski & Speziale (1993); (o) RDT (Rogers 1991).
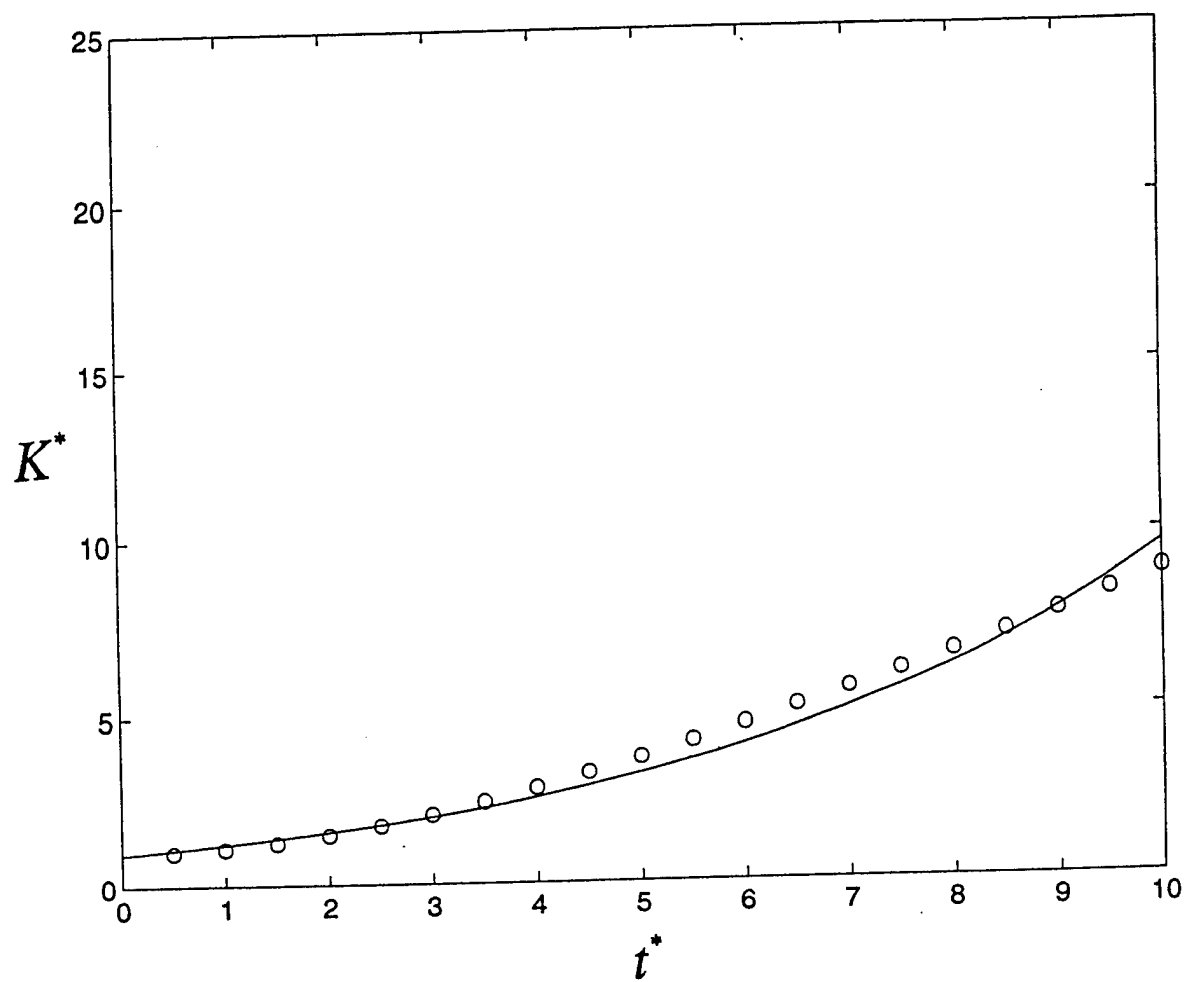
Figure 3.   Comparison of the model predictions of the new non-equilibrium ASM (—) for $SK_0 / \varepsilon_0 = 50$ with RDT (Rogers 1991) (o): time evolution of the turbulent kinetic energy in homogeneous shear flow.
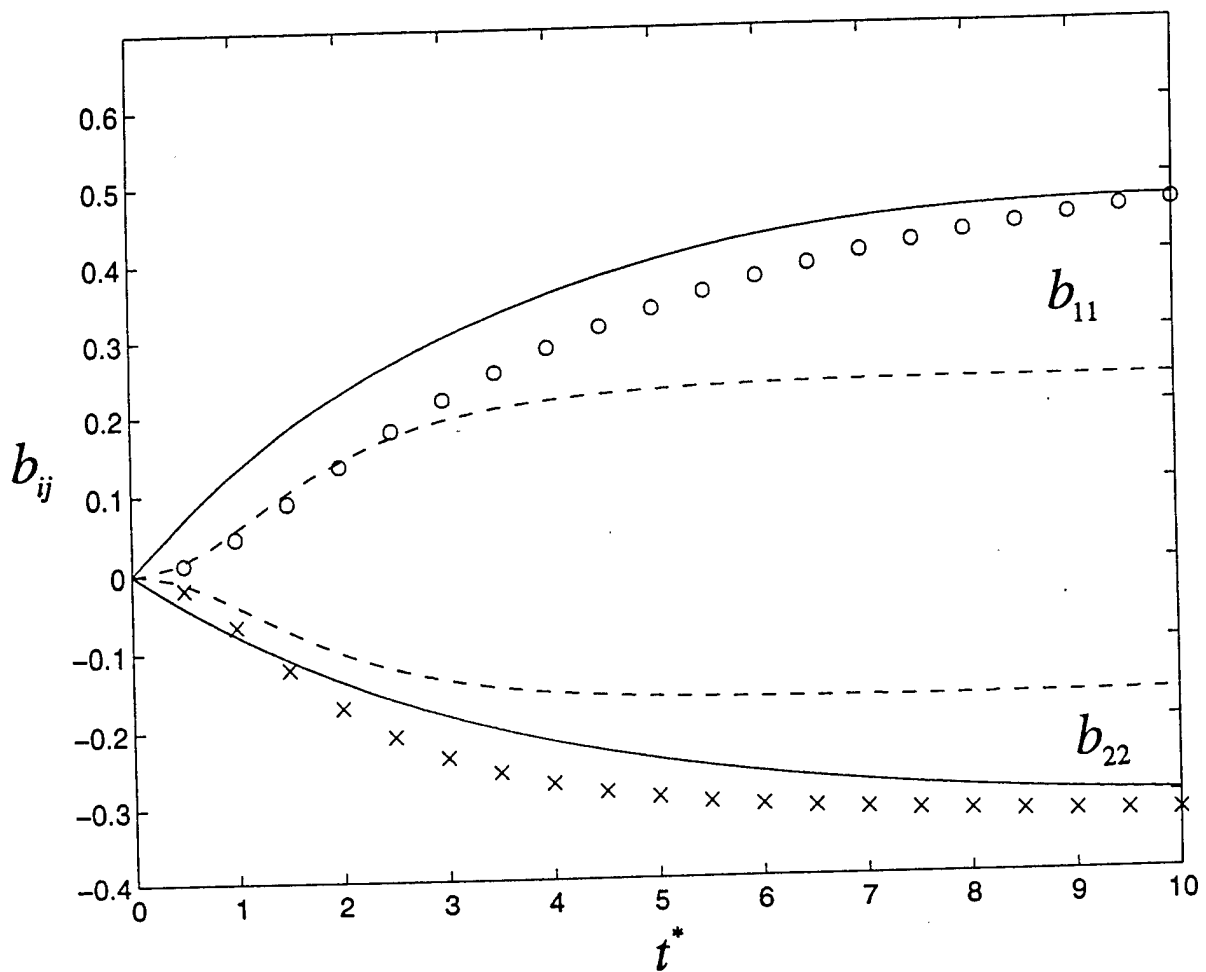
Figure 4. Time evolution of the Reynolds stress anisotropies in homogeneous shear flow: Comparison of the model predictions for $SK_0 / \varepsilon_0 = 50$ with Rapid Distortion Theory. (- - -) SSG Model; (——) New Relaxation Model; (o, ×) RDT (Rogers 1991).
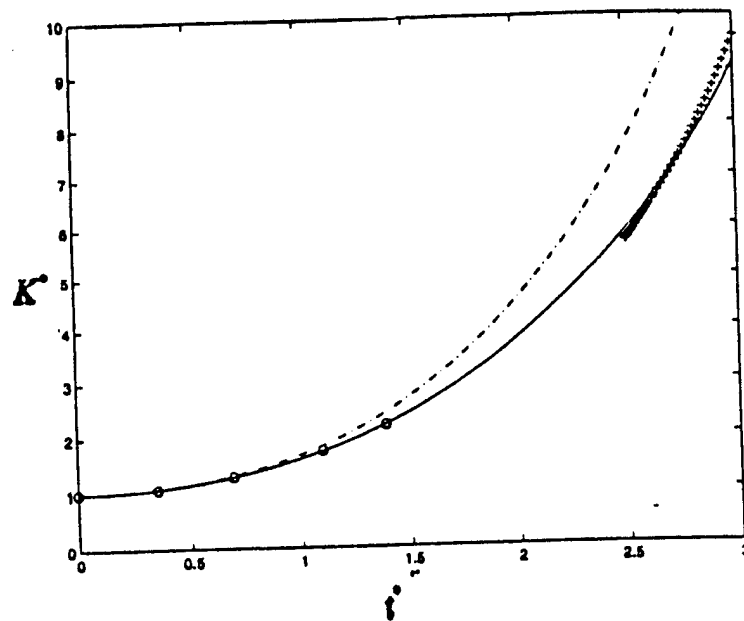
Figure 5. Growth rate of the turbulent kinetic energy in plane strain turbulence: Predictions of the new relaxation model. (— New model; - - - Equilibrium model; o DNS; × RDT).
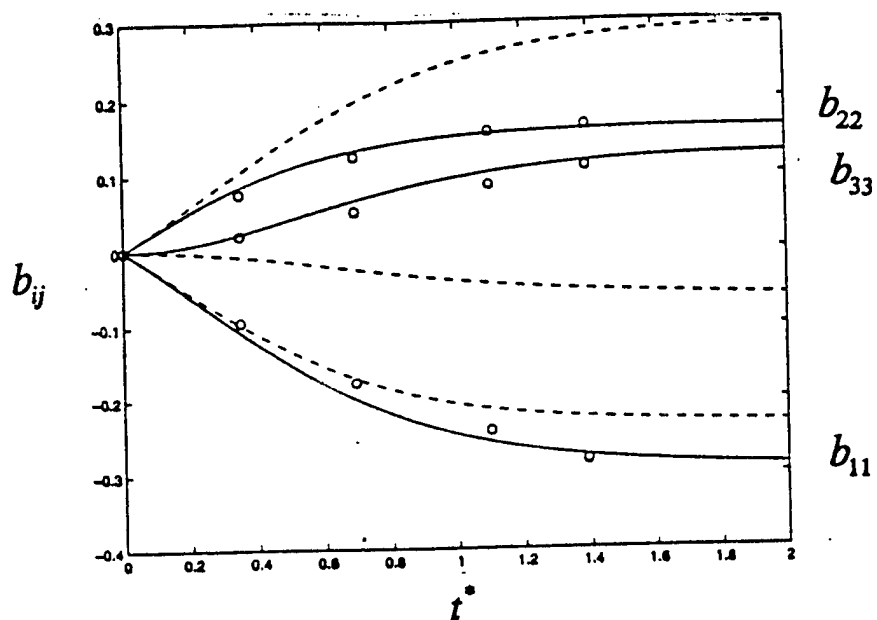
Figure 6. Growth of the Reynolds stress anisotropies in plane strain turbulence: Predictions of the new relaxation model. (— New model; - - - Equilibrium Model; o DNS).
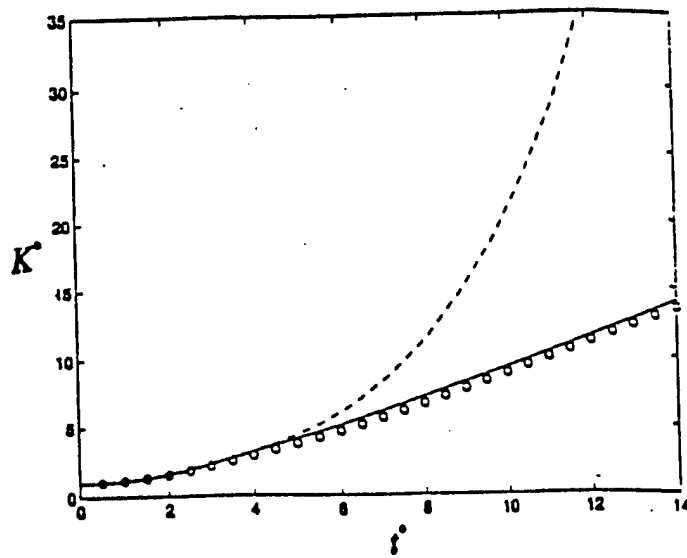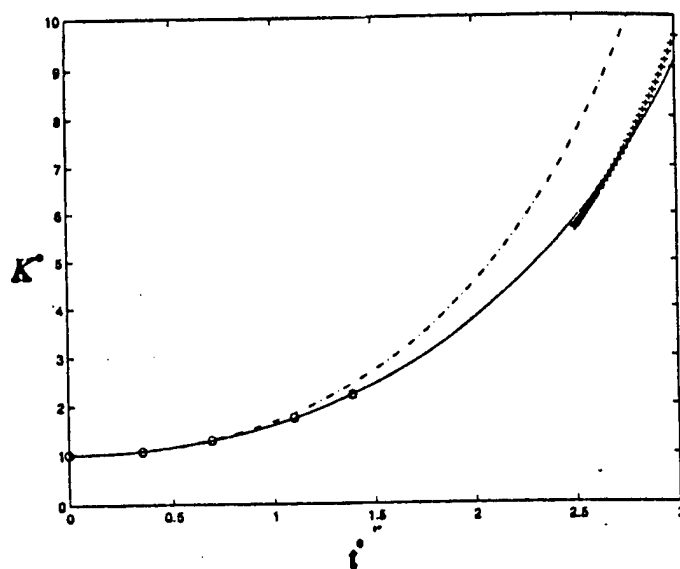
Figure 7. Predictions of the new non-equilibrium SSG second-order closure for the growth rate of the turbulent kinetic energy in homogeneous shear flow (— New Model; - - - Equilibrium Model; o RDT).
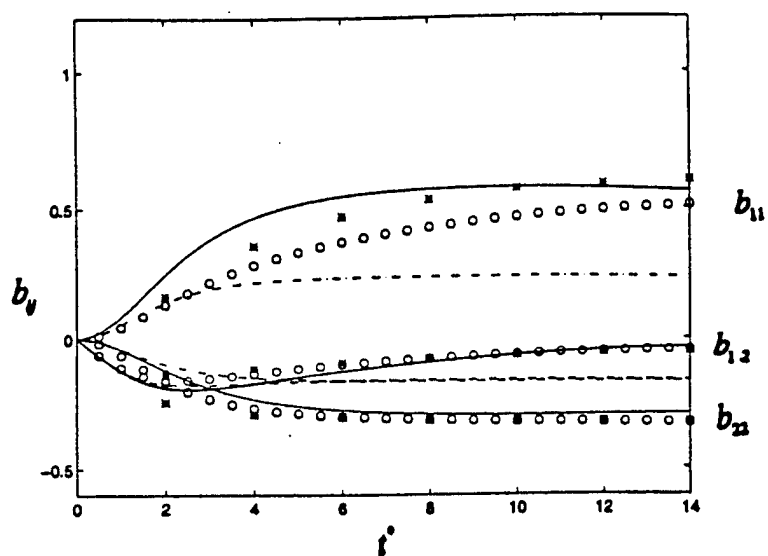
Figure 8. Predictions of the non-equilibrium SSG second-order closure for the Reynolds stress anisotropies in homogeneous shear flow (— New Model; * DNS; o RDT).

Figure 9. Predictions of the new non-equilibrium SSG second-order closure for the growth rate of the turbulent kinetic energy in plane strain turbulence (— New Model; - - - Equilibrium Model; o DNS; × RDT).
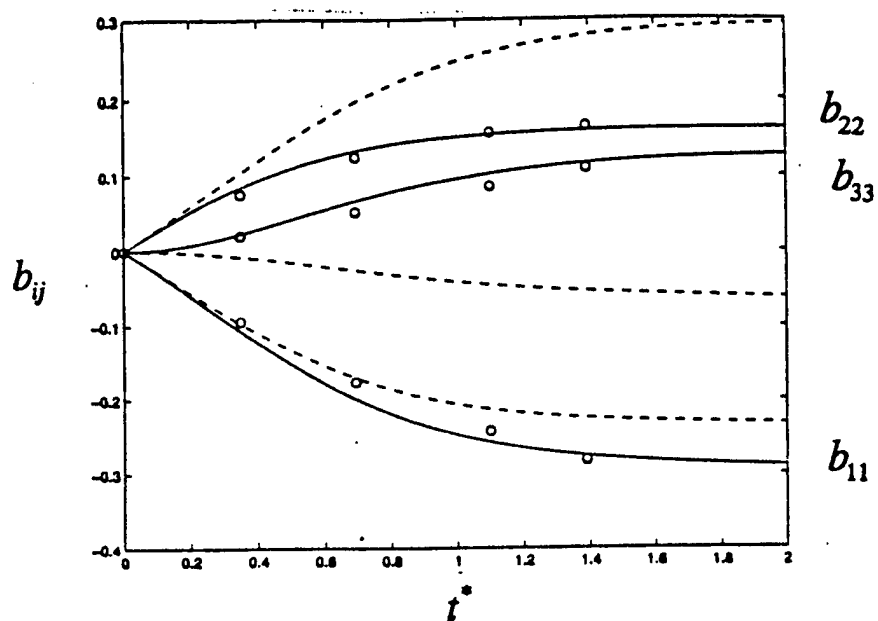
Figure 10. Predictions of the new non-equilibrium SSG second-order closure for the growth of the Reynolds stress anisotropies in plane strain turbulence (— New Model; - - - Equilibrium Model; o RDT).
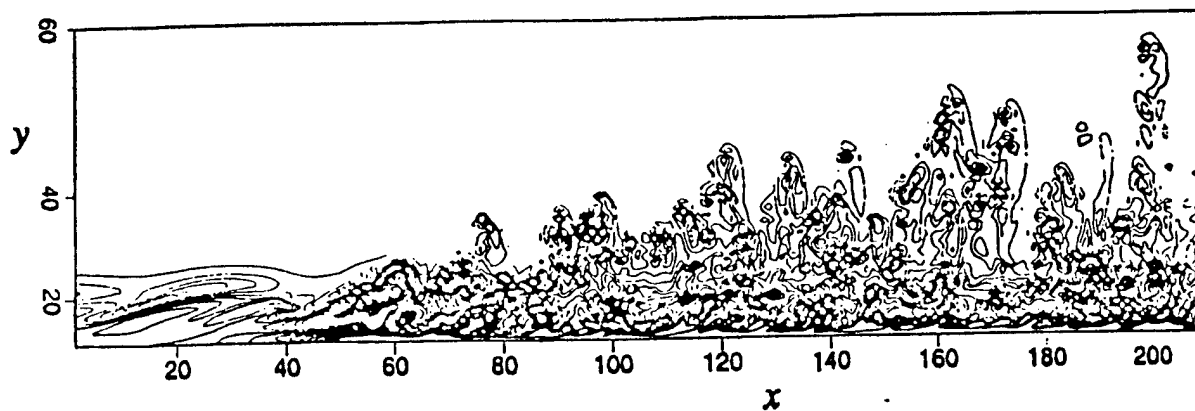
Figure 11. Plot of spanwise vorticity in the developing turbulent boundary layer obtained from LES (computations done by H. Fasel and co-workers at the University of Arizona).
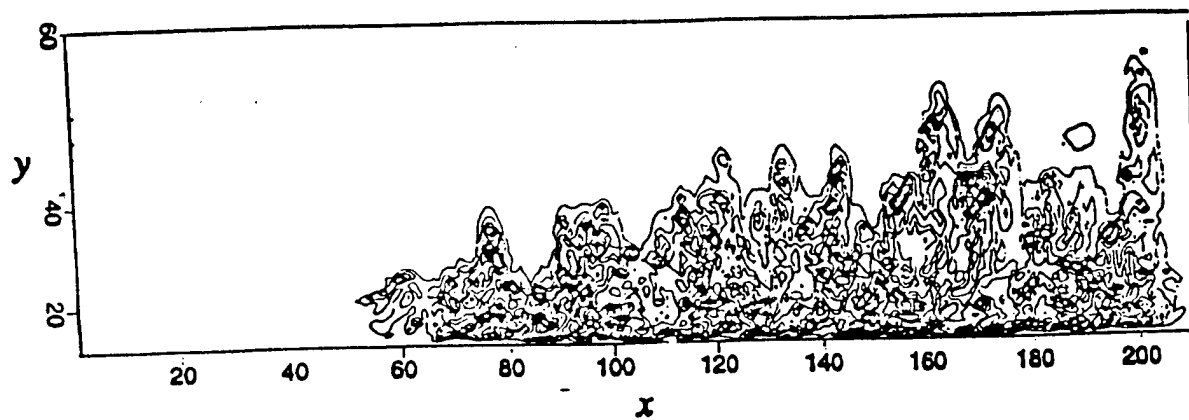
Figure 12. Plot of the eddy viscosity in the developing turbulent boundary obtained from LES (computations done by H. Fasel and co-workers at the University of Arizona).